Simulation of Alloy Oxidation

Simon R. Phillpot and Dieter Wolf (ANL-MSD)

OBJECTIVES

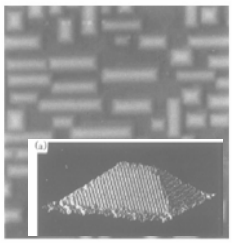
- To use atomic-level and mesoscale simulations to gain insights into the processes involved in oxidation.

- To deconvolute the strongly coupled effects present in experiment

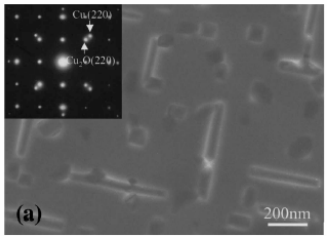
ULTIMATE GOAL

- To develop a phenomenological framework within which to explore and understand oxidation

EARLY-STAGE: ISLAND FORMATION AND RELATIONSHIP TO EPITAXY



Ge/Si, Mo et al.



Cu_2O/Cu(100), Zhou and Yang

- Island formation in Cu_2O/Cu similar to epitaxial Ge/Si

KEY ISSUES

- Crystal shape theory for epitaxial islands
- Surface energy anisotropy for Cu_2O on Cu
- Cu_2O/Cu interface energy
- Anisotropy in shape of Cu_2O islands on Cu as a function of T
- Competition between layer-by-layer growth and island formation

APPROACH

Molecular-dynamics simulations

Variable charge method of Streitz and Mintmire

INTERMEDIATE STAGE: MICROSTRUCTURE FORMATION BY ISLAND GROWTH AND COALESCENCE

KEY ISSUES

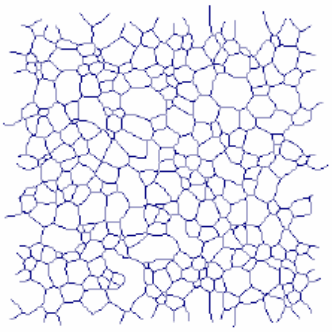
- How do the island shapes evolve as they start to impinge?
- Does the morphology of the newly grown layer echo that of the islands?
- What are the effects of stress?

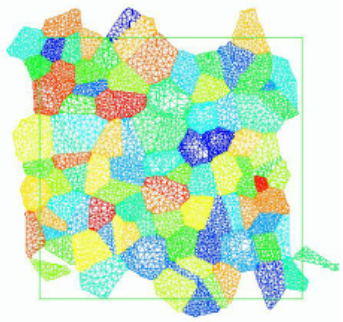
APPROACH

Mesoscale simulation using front tracking

- surface diffusion
- oxygen deposition

MESOSCALE SIMULATION OF EVOLUTION OF OXIDE LAYER





Combined front-tracking and continuum-elasticity approach

- Needleman-Rice Principal of virtual power dissipation

- Time scale set by grain-boundary processes

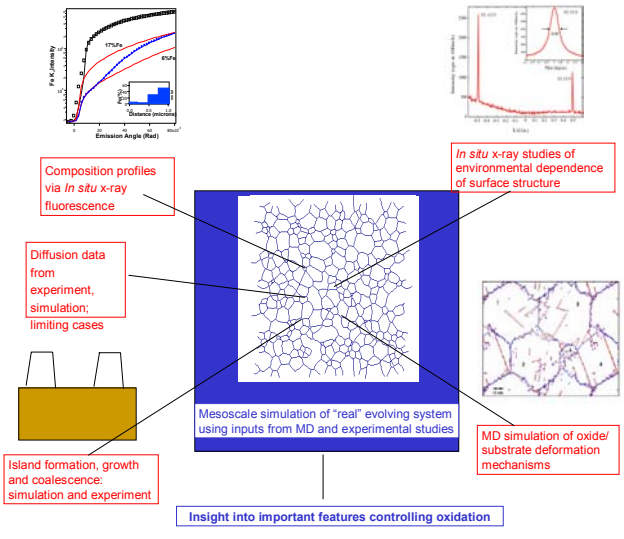
- Length scale set by grain size

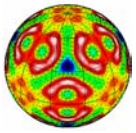
- Grain interiors meshed to account for inhomogeneous stress distribution

- Discretized grain boundaries

- Dynamics determined by grain and grain boundary properties

TOWARDS A PREDICTIVE MODEL OF ALLOY OXIDATION





BES - DOE

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